Furan, 2-[(2-furyl)-(4-bromophenylamino)methylcarbonyl

Inchi: InChI=1S/C16H12BrNO3/c17-11-5-7-12(8-6-11)18-15(13-3-1-9-20-13)16(19)14-4-2-10-2

InchiKey: BGDXKQNNEOSTAN-UHFFFAOYSA-N

Formula: C16H12BrNO3

SMILES: O=C(c1ccco1)C(Nc1ccc(Br)cc1)c1ccco1

Mol. weight [g/mol]: 346.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.07		Crippen Method
logp	4.671		Crippen Method
mcvol	214.410	ml/mol	McGowan Method
rinpol	2439.00		NIST Webbook
rinpol	2439.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R121183&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.